Tycho 2 User Guide (Draft)

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1 Introduction

Tycho 2 is a reworking of a code named Tycho written by Shawn Pautz around the year 2000. The original code solved a linear, kinetic, transport equation on an unstructured, 3D tetrahedral mesh and was parallelized via MPI. The original code was made to test the performance of transport sweeps which will be subsequently described.

Tycho 2 solves the same equation with some additions. The new code adds energy dependence to the calculations to give realistic computational results for cases with several energy groups. The code is implemented in MPI and OpenMP and uses only open source software and libraries to generate meshes and compile.

2 Compiling and running the code

The code is split into the main executable named `sweep.x` and several utilities dealing with meshes in the `util` directory. All the code requires a C++11 compliant compiler. The utilities require nothing more as they are written for serial code. The main program, sweep.x, also requires MPI and OpenMP to compile.

2.1 Compiling sweep.x

Quick step guide

- Copy `make.inc.example` to `make.inc`
- Set `ASSERT` and `MPICC` in the file `make.inc`
- Type `make` to build `sweep.x`

Details To compile `sweep.x`, first copy `make.inc.example` to `make.inc`. The file `make.inc` will contain the two user definable parts for the build process. The first user definable attribute is `ASSERT`. If `ASSERT = 1`, then the code will run much slower since bounds checking is performed on all the multidimensional arrays.

The second user definable parameter is your compiler information, which is set in `MPICC`. In this, you name the MPI compiler wrapper and any features of the compilation you want such as optimization and debugging symbols. You must enable C++11 and OpenMP for your compiler. For an optimized compile using GCC, I usually set `mpic++ -O3 -Wall -Wextra -pedantic`

`-std=c++11 -fopenmp`. This compile command is optimized to level 3, spits out as many warnings as possible, enables C++11 features, and enables OpenMP.

The last step is to type `make` to build the main executable.

3 The underlying mathematics

3.1 The equation

Tycho 2 solves the following kinetic equation with isotropic scattering

$$\Omega \cdot \nabla_x \Psi(x, \Omega, E) + \sigma_t \Psi(x, \Omega, E) = \frac{\sigma_s}{4\pi} \int_{\mathbb{S}^2} \Psi(x, \Omega', E) d\Omega' + Q(x, \Omega, E). \tag{1}$$

The function Ψ is the unknown, σ_t and σ_s are the total and scattering cross sections with $\sigma_t > \sigma_s$ and are constant. The function Q is a known source.

The independent variables are:

- Space – $x \in \mathcal{D} \subset \mathbb{R}^3$,
- Direction – $\Omega \in \mathbb{S}^2$ (the unit sphere),
- Energy – $E \in \mathbb{R}^{\geq 0}$.

Notice the equation is dependent on energy, but the different energies are not coupled. This is done on purpose since the goal is to test sweeping strategies which are uncoupled in energy.

For the purpose of simpler notation, define

$$\Phi(x, E) = \int_{\mathbb{S}^2} \Psi(x, \Omega', E) d\Omega' \tag{2}$$

to get the equivalent equation

$$\Omega \cdot \nabla_x \Psi(x, \Omega, E) + \sigma_t \Psi(x, \Omega, E) = \frac{\sigma_s}{4\pi} \Phi(x, E) + Q(x, \Omega, E). \tag{3}$$

3.2 Method of discretization

Equation (3) is discretized using: discontinuous Galerkin (DG) with linear elements in x, discrete ordinates in Ω, and energy groups in E.

Energy discretization. Since equation (3) is not coupled in energy, the method of discretization of E does not matter. However, it is typical to discretize E into energy groups. Hence, the discretization in energy is denoted by E_g where g is an integer indexing the energy group (though any other discretization is fine).

$$\Omega \cdot \nabla_x \Psi_g(x, \Omega) + \sigma_t \Psi_g(x, \Omega) = \frac{\sigma_s}{4\pi} \int_{\mathbb{S}^2} \Psi_g(x, \Omega') d\Omega' + Q_g(x, \Omega). \tag{4}$$

Angle discretization. Angle is discretized via discrete ordinates, which is often denoted as S_N where N is the order of the discretization. Tycho 2 implements the Chebyshev-Legendre quadrature of the sphere. This involves a Cartesian product of N Legendre nodes on the z-axis and $2N$ equally spaced points on the circle for each Legendre node. The weights are proportional to the weights of the Legendre quadrature and scaled to sum to 4π. The nodes and weights will be denoted by Ω_q and w_q, where q stands for the quadrature index.

Equation (1) becomes

$$\Omega_q \cdot \nabla_x \Psi_{qg}(x) + \sigma_t \Psi_{qg}(x) = \frac{\sigma_s}{4\pi} \sum_{q'=0}^{2N^2-1} w_{q'} \Psi_{q'g}(x) + Q_{qg}(x). \tag{5}$$

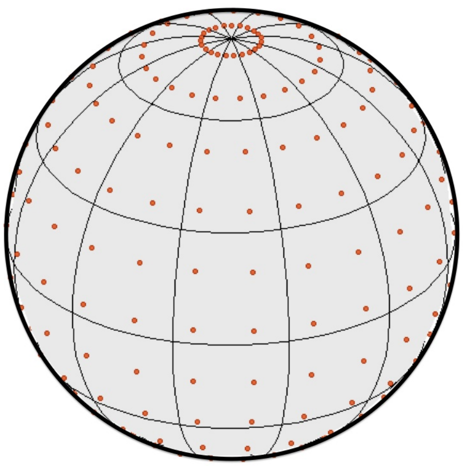
Equation (3) becomes

$$\Omega_q \cdot \nabla_x \Psi_{qg}(x) + \sigma_t \Psi_{qg}(x) = \frac{\sigma_s}{4\pi} \Phi_g(x) + Q_{qg}(x), \tag{6}$$

where

$$\Phi_g(x) = \sum_{q'=0}^{2N^2-1} w_{q'} \Psi_{q'g}(x). \tag{7}$$

Below is a depiction of the quadrature nodes on the sphere.



Spatial discretization. Since source iteration is used to converge the RHS of equation (1), it will be easier to show the equations for the simpler problem

$$\Omega_q \cdot \nabla_x \Psi_{qg}(x) + \sigma_t \Psi_{qg}(x) = Q_{qg}(x). \tag{8}$$

In this formulation, the scattering term has been absorbed into the source $Q_{qg}(x)$.

Space is discretized via linear DG. In each tetrahedral cell C_i, define basis functions $b_{ik}|_{k=0}^{3}$ to be linear interpolation functions with

$$b_{ik} = \begin{cases} 1, & \text{at vertex } k \text{ of cell } C_i \\ 0, & \text{at other vertices of cell } C_i \end{cases}. \tag{9}$$

Also, define

$$\Psi^h|_{C_i} = \sum_k \Psi_{ik} b_k. \tag{10}$$

Then the DG formulation is derived by starting with the equation

$$\Omega \cdot \nabla_x \Psi(x) + \sigma_t \Psi(x) = Q(x), \tag{11}$$

where the subscripts q, g are implicit. Then multiply by test function b_j in cell C_i and integrate to get

$$\int_{C_i} \Omega \cdot \nabla_x \Psi b_j dx + \int_{C_i} \sigma_t \Psi b_j dx = \int_{C_i} Q b_j dx. \tag{12}$$

Then use integration by parts on the first integral to get

$$-\int_{C_i} \Omega \cdot \nabla_x b_j \Psi dx + \sum_k \int_{F_{ik}} (\Omega \cdot \nu_k) b_j \hat{\Psi}^{(k)} dA + \int_{C_i} \sigma_t \Psi b_j dx = \int_{C_i} Q b_j dx. \tag{13}$$

Here, k indexes over the faces F_{ik} of cell i, and ν_k is the outward normal to face F_{ik}. The only thing left to define is the numerical flux $\hat{\Psi}^{(k)}$. Since Ψ is discontinuous at the faces, this is not well defined and must be defined by the numerical method. We use the upwind flux

$$\hat{\Psi}^{(k)} = \begin{cases} \Psi|_{F_{ik}} \text{ from } C_i, & \text{if } \Omega \cdot \nu_k > 0 \\ \Psi|_{F_{ik}} \text{ from adjacent cell}, & \text{if } \Omega \cdot \nu_k < 0 \end{cases} \tag{14}$$

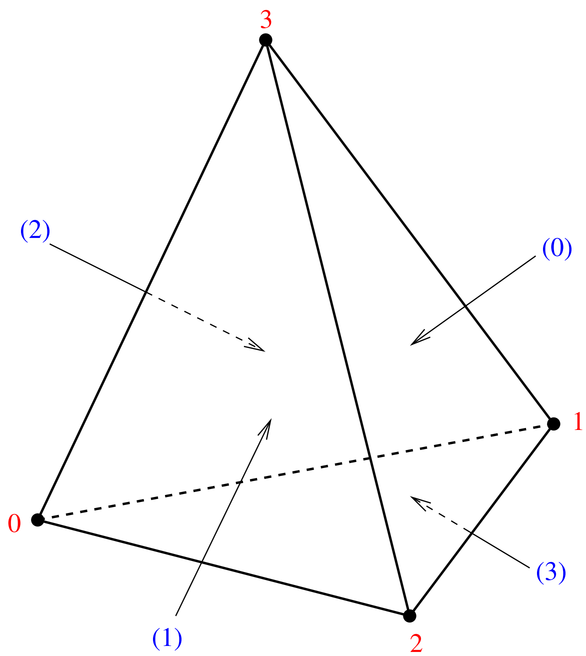
Putting everything together, one gets the linear system below. The derivation is described in an accompanying document. Face k is defined to be opposite vertex k as shown in the figure.

$$\begin{aligned} &\frac{1}{12}\bar{A}_1 \left(2\hat{\Psi}_0^{(1)} + \hat{\Psi}_2^{(1)} + \hat{\Psi}_3^{(1)}\right) + \frac{1}{12}\bar{A}_2 \left(2\hat{\Psi}_0^{(2)} + \hat{\Psi}_1^{(2)} + \hat{\Psi}_3^{(2)}\right) + \frac{1}{12}\bar{A}_3 \left(2\hat{\Psi}_0^{(3)} + \hat{\Psi}_1^{(3)} + \hat{\Psi}_2^{(3)}\right) \\ &+\frac{1}{12}\bar{A}_0 \left(\Psi_0 + \Psi_1 + \Psi_2 + \Psi_3\right) + \frac{\sigma_t V}{20} \left(2\Psi_0 + \Psi_1 + \Psi_2 + \Psi_3\right) = \frac{V}{20} \left(2Q_0 + Q_1 + Q_2 + Q_3\right) \end{aligned}$$

$$\begin{aligned} &\frac{1}{12}\bar{A}_0 \left(2\hat{\Psi}_1^{(1)} + \hat{\Psi}_2^{(1)} + \hat{\Psi}_3^{(1)}\right) + \frac{1}{12}\bar{A}_2 \left(\hat{\Psi}_0^{(2)} + 2\hat{\Psi}_1^{(2)} + \hat{\Psi}_3^{(2)}\right) + \frac{1}{12}\bar{A}_3 \left(\hat{\Psi}_0^{(3)} + 2\hat{\Psi}_1^{(3)} + \hat{\Psi}_2^{(3)}\right) \\ &+\frac{1}{12}\bar{A}_1 \left(\Psi_0 + \Psi_1 + \Psi_2 + \Psi_3\right) + \frac{\sigma_t V}{20} \left(\Psi_0 + 2\Psi_1 + \Psi_2 + \Psi_3\right) = \frac{V}{20} \left(Q_0 + 2Q_1 + Q_2 + Q_3\right) \end{aligned}$$

$$\begin{aligned} &\frac{1}{12}\bar{A}_0 \left(\hat{\Psi}_1^{(1)} + 2\hat{\Psi}_2^{(1)} + \hat{\Psi}_3^{(1)}\right) + \frac{1}{12}\bar{A}_1 \left(\hat{\Psi}_0^{(2)} + 2\hat{\Psi}_2^{(2)} + \hat{\Psi}_3^{(2)}\right) + \frac{1}{12}\bar{A}_3 \left(\hat{\Psi}_0^{(3)} + \hat{\Psi}_1^{(3)} + 2\hat{\Psi}_2^{(3)}\right) \\ &+\frac{1}{12}\bar{A}_2 \left(\Psi_0 + \Psi_1 + \Psi_2 + \Psi_3\right) + \frac{\sigma_t V}{20} \left(\Psi_0 + \Psi_1 + 2\Psi_2 + \Psi_3\right) = \frac{V}{20} \left(Q_0 + Q_1 + 2Q_2 + Q_3\right) \end{aligned}$$

$$\begin{aligned} &\frac{1}{12}\bar{A}_0 \left(\hat{\Psi}_1^{(1)} + \hat{\Psi}_2^{(1)} + 2\hat{\Psi}_3^{(1)}\right) + \frac{1}{12}\bar{A}_1 \left(\hat{\Psi}_0^{(2)} + \hat{\Psi}_2^{(2)} + 2\hat{\Psi}_3^{(2)}\right) + \frac{1}{12}\bar{A}_2 \left(\hat{\Psi}_0^{(3)} + \hat{\Psi}_1^{(3)} + 2\hat{\Psi}_3^{(3)}\right) \\ &+\frac{1}{12}\bar{A}_3 \left(\Psi_0 + \Psi_1 + \Psi_2 + \Psi_3\right) + \frac{\sigma_t V}{20} \left(\Psi_0 + \Psi_1 + \Psi_2 + 2\Psi_3\right) = \frac{V}{20} \left(Q_0 + Q_1 + Q_2 + 2Q_3\right) \end{aligned}$$



3.3 Source iteration

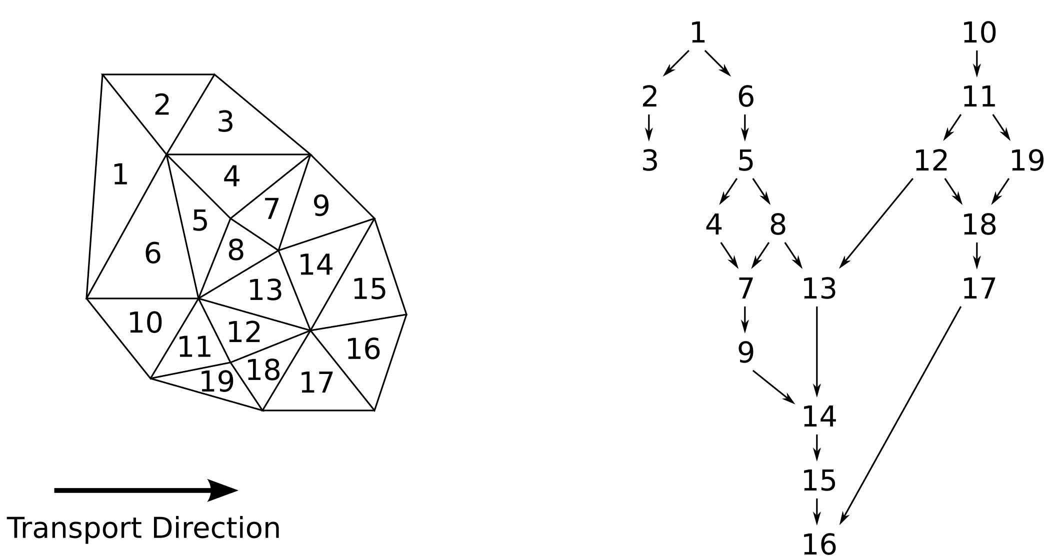
The overall algorithm is to lag the data from the integral on the RHS of equation (3). This is called source iteration

$$\Omega \cdot \nabla_x \Psi^{k+1} + \sigma_t \Psi^{k+1} = \frac{\sigma_s}{4\pi}\Phi^k + Q. \tag{15}$$

Tycho 2 iterates this process until $||\Phi^{k+1} - \Phi^k||_\infty / ||\Phi^{k+1}||_\infty <$ tolerance.

3.4 Sweeps

The most common method of solving the discretized form of equation (11) for Ψ is called a sweep. Consider the following 2D example shown below.



The sweep algorithm for the transport direction (angle) shown, shows that cells 1 and 10 have no dependencies except for the incoming boundary. Once Ψ is computed in these cells, the upwind flux is calculated for the boundaries between (1,2), (1,6), and (10,11). With this boundary data between cells known, Ψ in cells 2, 6, and 11 can be computed. This continues until Ψ is computed in all cells.

A sweep is needed for each angle and energy group. Fortunately, all these sweeps are completely independent and therefore trivially parallelizable.